

Supercomputers tackle antibiotic resistance

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Understanding antibiotic resistance starts with understanding bacteria. Bacteria are tiny single-celled organisms found nearly everywhere on Earth. Most bacteria are harmless to humans. Some are helpful. Some cause disease. Over millennia, bacteria have evolved ways to keep out harmful foreign substances. Many so-called Gram-negative bacteria, which have two cellular membranes, have evolved protein structures called efflux pumps that are lodged between the membranes and expel toxins out of the cell.

But what happens when the bacteria in question are the dangerous, disease-causing kind? Doctors try to kill them with antibiotics. But the dangerous bacteria often use efflux pumps to flush out antibiotics before the drugs get a chance to work.

One type of efflux pump, which until recently had only been studied piecemeal, was modeled in its entirety and simulated using supercomputers at Los Alamos National Laboratory. The work harnessed the laboratory's extensive modeling and supercomputing simulation capabilities developed in support of its national security mission.

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